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13. ABSTRACT (Maximum 200 words) AASERT supported work on the following: Modeling of multiple layer stacks in thin film growth; Modeling of energy input terms in electromagnetic excitation of materials; PRS monitoring of multiple layer stacks in thin film growth; construction and testing of a prototype high pressure organometallic chemical vapor deposition (HPOMCVD) reactor; Reduced order surface kinetic models for GaP growth; computational methods for feedback control in nonlinear systems.					
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Modeling Validation and Control of Advanced Chemical Vapor Deposition Processes

FINAL TECHNICAL REPORT for the period

September 1, 1996 - August 31, 1999

AFOSR F49620-96-1-0292 (AASERT)
Parent Award is AFOSR F49620-95-1-0447

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Objectives

The objective of this AASERT was to train three additional students under an existing DoD AFOSR MURI Center in Intelligent Design and Manufacturing in Electronics and Materials, DoD/AFOSR MURI F 49620-95-1-0447, entitled "Modeling and Control of Advanced Chemical Vapor Deposition Processes: The Control of Defects in Mixed III-V Compound Heterostructures". The students were trained in a multidisciplinary field of study that includes Materials Science and Engineering, Chemical Engineering, Applied Mathematics and Physics. The DoD-AFOSR MURI Center at North Carolina State University includes the above four disciplines and close collaborations with the Department of Materials Science and Engineering at Arizona State University. NCSU's Solid State Minor provides for the addition of selected courses in solid state science outside the student's major field of study. Thus the AASERT students had access to a broad base of training in science and engineering. The students who received AASERT support worked closely with Prof. K.J. Bachmann and Prof. H.T. Tran. The research of the students addressed topics that augment the PI's program in the context of the DoD AFOSR MURI Center, extending the scope of this program to new exciting areas of research that enhanced the impact of the Center's activities in science and technology.

Status of Efforts

Understanding surface chemistry under steady-state epitaxial growth involving organometallic chemical precursor molecules is essential for optimizing growth processes. One specific method, p-polarized reflectance spectroscopy (PRS), is very well suited for this task as its application is not limited to a high vacuum environment. The simplest possible description of the optical response under the conditions of chemical vapor deposition is based on a four-layer stack: ambient-surface reaction layer-epilayer-substrate. This four-layer stack Fresnel formula is derived from the Maxwell equations.

Working with scientists and engineers in the MURI interdisciplinary team, students developed a MATLAB module implementing the Fresnel formula. In addition, they also wrote several MATLAB modules to analyze the experimental data including automatically removing undesirable data points and to perform least-squares fit of data with the model.

Working with faculty advisors, students investigated the energy input in electromagnetic excitation of materials. In particular, they studied basic level polarization assumptions underlying standard input terms derived in the literature using first principles and Maxwell's equations.

Students also assisted MURI team members in four specific tasks:

1. Development of inverse problem algorithms being used in analysis of PRS responses in monitoring heteroepitaxial GaP growth.

2. Construction and early testing of an HPOMCVD reactor that was a main objective of this MURI grant.
3. Development of reduced order surface kinetic models to be used in heteroepitaxial GaP growth on Si.
4. Development of computational methods for feedback control in non-linear systems.

Accomplishments and New Findings

1. Real time monitoring with PRS

The team continued to explore the application of p-polarized reflectance spectroscopy (PRS) for the real time monitoring and control of pulsed chemical beam epitaxy (PCBE). Control of the growth process using the optical signature from the surface reaction layer (SRL) that feeds the underlying growth requires detailed instantaneous simulation and prediction of the surface chemistry and its link to the optical properties of the outer most layer in a multilayer stack. In this context, using heteroepitaxial GaP growth as an example, the team successfully introduced a reduced order kinetic model to describe the growth process and, in turn, demonstrated the linkage of the PRS response towards surface reaction chemistry, composition, film growth rate, and film properties. Formulated as an inverse least squares problem, unknown parameters in the mathematical model (e.g., reaction rates, optical responses) were computed to give a very good match between the mathematical model and the data provided by the PRS measurement.

2. Construction and testing of the HPOMCVD reactor

The AASERT stipend made available to us supported the work of Ms. Sonya McCall and the work of Ms. Stacie LeSure. Ms. Sonya McCall and a post-doc, Dr. Christian Höpfner, worked in 1997 on the construction of the high pressure OMCVD system that we built as part of the deliverables of DoD MURI F-4620-95-1-0447. Dr. Höpfner left us in April 1998 for a position with Spire Corporation, Bedford, MA. He was replaced by Dr. Fuchao Wang, who continued the collaboration with Ms. McCall to bring the system into full operation. It was put onto continuous purge gas flow in May 1998 and was tested and supplemented by additional safety precautions to confirm to safety rules established by the University. Ms. LeSure's work focused on early stages of heteroepitaxy, building upon the work of another graduate

student, who was supported by our DoD MURI grant, Mr. Nkadi Sukidi. Mr. Sukidi successfully defended his Ph.D. thesis in Materials Science and Engineering in Spring of 1998 and is now working at the Bipolar-One facility of Motorola Company at Mesa, AZ. Ms. LeSure participated in testing of the OMICRON ultra-high vacuum scanning tunneling microscope that we acquired in 1997 with funding by the above DoD MURI grant. Atomic resolution was obtained so that the vibrational damping in the laboratory, where this instrument is located suffices for the intended in-situ studies of nucleation and overgrowth mechanisms. By starting a collaboration with Prof. Russell, who contributed a focused ion beam column to the UHV-STM system, we were able to execute nanoscale machining tasks on heterostructures, grown in the high pressure OMCVD system and brought into the sample preparation chamber through a load-lock. Also, we assembled a sample preparation chamber that permitted chemical beam epitaxy processing and transfer of samples between the focused ion beam machining chamber and the UHV-STM chamber. This will enable work on advanced nanostructures, including materials that heretofore have not been available. The evaluation of microstructure by high resolution transmission electron microscopy supplementing the STM studies was continued in cooperation with Prof. Mahajan. Ms. LeSure spent some time in Prof. Mahajan's laboratory, so that the close collaboration with his students continued at optimum output.

3. Reduced order surface kinetic model

We developed a reduced order surface kinetic model using generalized reaction rate parameters to describe the decomposition kinetics of the organometallic precursors TBP and TEG used during heteroepitaxial growth of GaP on Si. The set of coupled differential equations that describe the surface reaction kinetics provide information about the dynamics of molar concentrations of precursor fragments stored in the surface reaction layer and their incorporation into the underlying growth film. We successfully fitted sets of experimental data using this model to identify the unknown parameters involved in the surface kinetics and their effect on the polarized-reflectance measurements. The results positively showed that the mathematical model can be used to effectively predict the large- and small-scale features of the experimental data and to model the deposition process. Significant efforts and progress were made on computational methods for the design and synthesis of feedback controls for nonlinear systems. In particular, we made a very comprehensive comparison study of several methods proposed in the literature which include the power series approximation to the Hamilton Jacobi Bellman (HJB) equation, state-dependent Riccati

equation, successive Galerkin approximation, and methods based on interpolation of open-loop controls into closed-loop forms. The results of this study significantly impacted our MURI efforts on developing feedback controls and compensators design for high pressure chemical vapor deposition (HPCVD) reactor.

Personnel Supported

S. Beeler, S. McCall, N. Young, C. Cole, M. Joyner and S. LeSure

Publications

1. K.J. Bachmann, N. Sukidi, C. Höpfner, C. Harris, N. Dietz, H.T. Tran, S. Beeler, K. Ito and H.T. Banks, "Real-time monitoring of steady-state pulsed chemical beam epitaxy by p-polarized reflectance", *J. Cryst. Growth*, **183** (1998) pp. 323-337.
2. K.J. Bachmann, S. McCall, S. LeSure, N. Sukidi and F. Wang, "Chemical deposition at high pressure in a microgravity environment", *Jpn. J. of Microgravity Sci.*, (1998) to appear.
3. S. Beeler, H.T. Tran and N. Dietz, "Representation of GaP formation by a reduced order surface kinetics model using p-polarized reflectance measurements", *J. of Applied Physics*, **86** (1999), pp. 674-682.
4. S. Beeler, H.T. Tran and H.T. Banks, "Feedback control methodologies for nonlinear systems", *J. Optimization Theory & Applic.*, to appear.

Interactions/Transitions

see parent grant

New Inventions/Patents

None

Honors and Awards

S.C. Beeler, NSF Graduate Fellow M. Joyner, NASA Graduate Fellow